

L^AT_EX

The equation of state and specific heat of the electron gas on a one dimensional lattice

Vladan Celebonovic

Institute of Physics,Pregrevica 118,11080 Zemun-Beograd,Yugoslavia

vladan@phy.bg.ac.yu
vcelebonovic@sezampro.yu

to appear in Phys.Low-Dim.Structures.,**1/2**,XXX (1999)

Abstract:Using previous results and general thermodynamical formalism,an expression is obtained for the specific heat per particle under constant volume of a degenerate non-relativistic electron gas on a 1D lattice.The result is a non-linear function of the temperature,and it could have applications in studies of quasi one-dimensional organic metals.

Introduction

The purpose of this paper is to determine the equation of state and specific heat of the electron gas on a one dimensional lattice. In experiments, the electronic specific heat is determined indirectly, only after somehow estimating and subtracting the phonon heat capacity from the measured heat capacity of the specimen. On the purely theoretical side, the electronic specific heat is directly related to the exact single particle Green's functions [1a]. The calculations, to be reported in the following section, are motivated by recent theoretical and experimental results on transport processes in quasi one-dimensional (Q1D) organic metals [1],[2]. A preliminary version of the calculation has already been published [3].

Q1D organic metals, later named the Bechgaard salts, were discovered in 1980 [4],[5]. It was experimentally shown soon afterwards that their transport properties are widely different from those of ordinary metals (for example [6] and references given there). For a general review of the field of organic conductors see [7].

The calculations

It will be assumed in the calculations that the number of particles N in the system is a variable. The starting point is a well known thermodynamical relation [8]

$$dG = -SdT + VdP + \mu dN \quad (1)$$

where $G = \mu N$ and all the symbols have their standard meanings. Inserting the definition of G into eq.(1), it follows that

$$-SdT + VdP + \mu dN = \mu dN + Nd\mu \quad (2)$$

Differentiating eq.(2) with respect to T gives

$$V(1 + \frac{1}{V} \frac{\partial V}{\partial T}) \frac{\partial P}{\partial T} = S + \frac{\partial S}{\partial T} + \frac{\partial N}{\partial T} \frac{\partial \mu}{\partial T} + N \frac{\partial \mu}{\partial T} \quad (3)$$

In the last equation we have used $dP = \frac{\partial P}{\partial T} dT$ and similar relations for other variables in eq.(2) .

Equation (3) is expressed in terms of the parameters of the system in bulk. Changing the variables to the number density n ($N = nV$) and the entropy per particle s ($S = nsV$) after some algebra one arrives at

$$V(1 + \frac{1}{V} \frac{\partial V}{\partial T}) \frac{\partial P}{\partial T} = ns(V + \frac{\partial V}{\partial T}) + V \frac{\partial n}{\partial T} (s + \frac{\partial \mu}{\partial T}) + nV \frac{\partial}{\partial T} (s + \mu) + n \frac{\partial \mu}{\partial T} \frac{\partial V}{\partial T} \quad (4)$$

We have thus obtained the EOS of any material in differential form. In applications to Q1D organic metals, it can be considerably simplified. Experiments on these materials are usually performed under constant volume [7]. This implies that all terms in eq.(4) containing derivatives of the volume can be disregarded. Accordingly, the final form of the EOS of Q1D organic metals is

$$\frac{\partial P}{\partial T} = (n + \frac{\partial n}{\partial T})(s + \frac{\partial \mu}{\partial T}) + n \frac{\partial s}{\partial T} \quad (5)$$

The specific heat per particle is given by [8]

$$c_V = \frac{T}{n} (\frac{\partial^2 P}{\partial T^2})_V - T (\frac{\partial^2 \mu}{\partial T^2})_V \quad (6)$$

Differentiating eq.(5), and inserting the result into eq.(6), gives the following final expression for the specific heat per particle

$$c_V = \frac{T}{n} (s + \frac{\partial \mu}{\partial T}) (\frac{\partial n}{\partial T} + \frac{\partial^2 n}{\partial T^2}) + \frac{T}{n} \frac{\partial n}{\partial T} (2 \frac{\partial s}{\partial T} + \frac{\partial^2 \mu}{\partial T^2}) + T (\frac{\partial s}{\partial T} + \frac{\partial^2 s}{\partial T^2}) \quad (7)$$

Discussion

Equation (7) is considerably more complex than the preliminary result already published in [3]. This difference is due several simplifying assumptions made in [3], which were dropped in the present paper. Basically, it was assumed there that the entropy per particle is temperature independent, that the total number of particles in the system is a constant, and the term $\frac{\partial n}{\partial T} \frac{\partial \mu}{\partial T}$ was neglected.

The aim of the calculation reported here was to obtain an expression for the differential form of the EOS and the specific heat ,but without all these simplifications.The result for the EOS is given by eq.(4).It was derived using general thermodynamical arguments,and accordingly can be applied to any material.In the special case of Q1D organic metals,one can introduce the constant volume condition into eq.(4) and thus obtain eqs.(5) and (7).

In application to the degenerate electron gas on a 1D lattice,one has to introduce into eq.(7) appropriate expressions for the chemical potential,number density and entropy per particle.It has recently been shown that the chemical potential of the electron gas on a 1D lattice is given by [9]

$$\mu = \frac{(\beta t)^6 (af - 1) |t|}{1.1029 + .1694(\beta t)^2 + .0654(\beta t)^4} \quad (8)$$

where a denotes the lattice constant, t the hopping, f the band filling and β the inverse temperature.The influence of the lattice is contained in this expression through the presence of the lattice constant a .

The entropy per electron and the number density should also be expressed so as to take into account the existence of the lattice.Work on this problem is currently in progress,but as a first approximation one could use existing results for the degenerate electron gas [10],[13] .The entropy per electron is given by

$$s = \frac{Q}{n_e} \frac{\partial}{\partial T} F_{3/2}(\beta\mu) \quad (9)$$

where $F_{3/2}(\beta\mu)$ is a special case of a Fermi-Dirac integral [10], n_e denotes the electronic number density,and Q is a combination of known constants (such as the electron mass and Planck's constant).The number density of a degenerate electron gas at low teemperature can be expressed in analytical form as [10]

$$n_e \cong AT^{15/2}[1 + BT^{3/2} +] \quad (10)$$

A, B again denote combinations of known constants.Inserting expressions (8) - (10) in eq.(7) one would get the final result for the specific heat of the electron gas on a 1D lattice.

How can eq.(7) be applied in the analysis of experimental data on Q1D organic metals? It can be used in analyzing data on the specific heat and thermal conductivity of these materials, such as those discussed in [1].

The specific heat of a solid can be decomposed into phonon and electronic parts. Their relative contributions to the "summary" specific heat of the specimen are functions of the parameters of the system. The most important of them are the temperature and the density. Expression (8) for the chemical potential was derived assuming that the Fermi liquid picture can be used for describing electrons in Q1D organic metals. This assumption is at present a subject of active discussion (see, for example, [11], [12]). Holding to this assumption, it then follows that eq.(7) can be applied to determining the phonon part of the specific heat from the experimental data. On the other hand, starting from the measured values of the specific heat, and the somehow theoretically estimated phonon contribution, one could obtain the electronic part. Comparing this function with the predictions of eq.(7), one could test the applicability of the Fermi liquid picture to electrons in Q1D organic metals.

The reasoning behind applications of eq.(7) to studies of the thermal conductivity of Q1D organic metals is essentially the same. It can be shown from elementary considerations [14] that the thermal conductivity is proportional to the specific heat. Taking eq.(7) in account, this implies that the thermal conductivity of Q1D organic metals is a nonlinear function of the temperature, in line with recent experiments [1]. Again, this could be used to test theoretical models of the organic metals. Work aiming at details of this comparison is currently in preparation.

Acknowledgement

This paper is dedicated to the memory of the late Heinz.J.Schulz from Laboratoire de Physique des Solides in Orsay (France) who introduced me to the field.

References

- [1] S.Belin and K.Behnia,Phys.Rev.Lett.,**79**,2125 (1997).
- [1a] C.M.Varma,preprint cond-mat/9607105 v2 (1996).
- [2] V.Celebonovic,Phys.Low-Dim.Struct.,**3/4**, 65 (1997)
and preprint cond-mat/9702147 .
- [3] V.Celebonovic,Solid State Phenomena,**61-62**,135 (1998c).
- [4] K.Bechgaard,C.S.Jacobsen,K.Mortensen et al.,Solid
State Comm.,**33**,1119 (1980).
- [5] D.Jerome,A.Mazaud,M.Ribault and K.Bechgaard,
C.R.Acad.Sc.Paris.,**B290** ,27 (1980);
D.Jerome,A.Mazaud,M.Ribault and K.Bechgaard,J.Physique
(Paris),Lettres,**41**,L95 (1980).
- [6] D.Jerome and F.Creuzet,in: Novel Superconductivity (ed.by
S.A.Wolf and V.Z.Kresin),p.103,Plenum Press, New York (1987).
- [7] T.Ishiguro and K.Yamaji,Organic Conductors,Springer Verlag,
Berlin (1990).
- [8] H.E.Stanley,Introduction to phase transitions and critical phenomena,
Clarendon Press,Oxford (1971).
- [9] V.Celebonovic,Phys.Low-Dim.Struct.,**11/12**,25 (1996)
and preprint cond-mat/9512016.
- [10] V.Celebonovic,Publ.Astron.Obs.Belgrade,**60**,16 (1998a)
and preprint astro-ph/9802279.
- [11] J.Voit,Rep.Progr.Phys.,**58**,975 (1995).
- [12] C.Bourbonnais,preprint cond-mat/9611064 v2 (1996);
A.Schwartz,M.Dressel,G.Grunner et al.,Phys.Rev.,**B58**,1261 (1998);
J.Moser,M.Gabay,P.Auban-Senzier,D.Jerome,K.Bechgaard
and J.M.Fabre,Eur.Phys.J.,**B1**, 39 (1998) .
- [13] L.D.Landau and E.M.Lifchitz,Statisticheskaya fizika,Vol.1,
Nauka,Moscow (1976).
- [14] N.W.Ashcroft and N.D.Mermin,Solid State Physics,
Holt,Rinehart and Winston,London (1976).